201-16166B

IUCLID

Data Set

Existing Chemical	:	ID: 620-22-4
CAS No.	:	620-22-4
EINECS Name	:	m-toluonitrile
EC No.	:	210-631-5
Molecular Formula	:	C8H7N

Producer related part

Company	:	Syngenta Crop Protection, Inc.
Creation date	:	16.09.2005

Substance related part

Company	:	Syngenta Crop Protection, Inc.
Creation date	:	16.09.2005
Status	:	
Memo	:	mtn.V2
Printing date	:	21.12.2005
Revision date	:	
Date of last update	:	21.12.2005
Number of pages	:	19
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

Type	:	cooperating company
Name	:	Syngenta Crop Protection, Inc.
Contact person	:	
Date	:	
Street	:	P.O. Box 18300
Town	:	NC 27419-8300 Greensboro
Country	:	United States
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	
Email	:	
Homepage	:	www.syngenta-us.com

21.12.2005

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

1.1.0 SUBSTANCE IDENTIFICATION

IUPAC Name	:	3-methylbenzonitrile
Smiles Code	:	C(#N)c(cccc1C)c1
Molecular formula	:	C8H7N
Molecular weight	:	117.15
Petrol class	:	

19.12.2005

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type	:	typical for an intermediate process substance
Substance type	:	Organic
Physical status	:	Liquid
Purity	:	> 99 % w/w
Colour	:	clear very slight yellow
Odour	:	none reported

16.09.2005

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

3-methylbenzonitrile	20.12.2005
3-Cyanotoluene	16.09.2005
3-Tolunitrile	16.09.2005
3-Tolyl cyanide	16.09.2005
m-Cyanotoluene	16.09.2005
m-Methylbenzonitrile	16.09.2005
m-Toluonitrile	16.09.2005
Metamethylbenzonitrile	16.09.2005
NSC 75453	16.09.2005

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

Type of use : Industrial
Category : chemical industry: (intermediate) used in synthesis

16.09.2005

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

16.09.2005

Type	:	EINECS
Additional information	:	No. 210-631-5
Type	:	ENCS
Additional information	:	No. 3-1804X
Type	:	other: SWISS
Additional information	:	No. G-5382
Type	:	TSCA
Additional information	:	January 2005 TSCA Inventory
Type	:	NDSL
Additional information	:	Canada Gazette, Part I, January 31, 1998
Type	:	other: ASIA-PAC
Additional information	:	

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

Type of search	:	Internal and External
Chapters covered	:	1, 2, 3, 4, 5
Date of search	:	16.09.2005

1.13 REVIEWS

2.1 MELTING POINT

Value	:	-23 °C
Sublimation	:	
Method	:	other: experimental
Year	:	2005
GLP	:	No
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Full citation not found.
Reliability	:	(2) valid with restrictions 2g: Data from Handbook or collection of data

20.12.2005 (1)

2.2 BOILING POINT

Value	:	213 °C
Decomposition	:	
Method	:	other: experimental
Year	:	
GLP	:	No
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Full citation not found.
Reliability	:	(2) valid with restrictions Data from Handbook or collection of data

20.12.2005 (1)

2.3 DENSITY

Type	:	Density
Value	:	9760 g/cm³
Method	:	
Year	:	
GLP	:	No
Test substance	:	
Reliability	:	(2) valid with restrictions Data from Handbook or collection of data

19.12.2005 (3)

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value	:	0.187 at 25 °C
Decomposition	:	
Method	:	other (calculated)
Year	:	2005
GLP	:	No
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Value calculated using EPA's programs. MPBPWIN v1.41. Mean of Antoine and Grain methods. Boiling point used 213 deg C
Reliability	:	(2) valid with restrictions 2f: Accepted calculation method

19.12.2005 (2)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	octanol-water
Log pow	:	2.087
pH value	:	
Method	:	other (calculated): KOWWIN v1.67
Year	:	2005
GLP	:	No
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Value calculated using EPA's programs.
Reliability	:	(2) valid with restrictions 2f: Accepted calculation method

19.12.2005 (2)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	921.2 mg/l at 25 °C
pH value	:	
concentration	:	
Temperature effects	:	
Examine different pol.	:	
pKa	:	
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: calculated KOWWIN V1.67
Year	:	2005
GLP	:	No
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Value calculated using EPA's programs.
Reliability	:	(2) valid with restrictions 2f: Accepted calculation method

19.12.2005 (2)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	Air
Light source	:	
Light spectrum	:	
Relative intensity	:	based on intensity of sunlight
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	1500000 molecule/cm³
Rate constant	:	0.0000000000008023 cm³/(molecule*sec)
Degradation	:	= 50 % after 13.3 day(s)
Deg. product	:	
Method	:	other (calculated): AOP Program (v1.91)
Year	:	2005
GLP	:	No
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Value calculated using EPA's programs.
Reliability	:	(2) valid with restrictions 2f: Accepted calculation method

19.12.2005 (2)

3.1.2 STABILITY IN WATER

Deg. product	:	
Method	:	other: (calculated) HYDROWIN v1.67
Year	:	2005
GLP	:	No
Test substance	:	as prescribed by 1.1 - 1.4
Remark	:	Not able to estimate a hydrolysis rate constant. Calulation not performed EPA method HYDROWIN (v1.67)

19.12.2005 (2)

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

Type	:	fugacity model level III
Media	:	other: air - water - soil - sediment
Air	:	% (Fugacity Model Level I)
Water	:	% (Fugacity Model Level I)
Soil	:	% (Fugacity Model Level I)
Biota	:	% (Fugacity Model Level II/III)
Soil	:	% (Fugacity Model Level II/III)
Method	:	other: Level III Fugacity Model
Year	:	2005
Method	:	Value calculated using EPA's programs.

Result : Level III Fugacity Model (Full-Output):

==========

Chem Name : Benzonitrile, 3-methyl-
Molecular Wt: 117.15
Henry's LC : 4.77e-005 atm-m3/mole (Henrywin program)
Vapor Press : 0.187 mm Hg (Mpbpwin program)
Log Kow : 2.09 (Kowwin program)
Soil Koc : 50.4 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	8.13	320	1000
Water	28.5	360	1000
Soil	63.3	720	1000
Sediment	0.111	3.24e+003	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	2.09e-010	217	1e+003	7.24	33.4
Water	7.15e-010	676	351	22.5	11.7
Soil	1.17e-008	752	0	25.1	0
Sediment	6.33e-010	0.294	0.0275	0.00979	0.000916

Persistence Time: 411 hr
Reaction Time: 750 hr
Advection Time: 911 hr
Percent Reacted: 54.9
Percent Advected: 45.1

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
Air: 319.9
Water: 360
Soil: 720
Sediment: 3240
Biowin estimate: 2.783 (weeks)

Reliability : (2) valid with restrictions
2f: Accepted calculation method

19.12.2005 (2)

3.3.2 DISTRIBUTION

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	3000 mg/kg bw
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	no data
Number of animals	:	
Vehicle	:	other:tragarth
Doses	:	not given
Method	:	
Year	:	1969
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Rats were dosed orally. The observation period was at least 7 days. Any surviving animals were killed and dissected after this time. No further details given
Result	:	LD50: The median lethal dose of 3-methylbenzonitrile when administered to rats is 3000 mg/kg.
Reliability	:	(3) invalid 3a: Documentation insufficient for assessment

20.12.2005 (4)

5.1.2 ACUTE INHALATION TOXICITY

Type	:	other: maximum tolerable exposure
Value	:	
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Exposure time	:	480 minute(s)
Method	:	
Year	:	1969
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Rats were exposure to saturated vapours of the test material. The method followed was cited to be a "saturation-time -test". Exposure time was judged to be such that all the animals survived a 7-day observation period. Surviving rats were then killed and dissected. No further details given
Result	:	The maximum tolerable exposure of 3-methylbenzonitrile when administered to rats is 480 minutes.
Reliability	:	(3) invalid 3a: Documentation insufficient for assessment

20.12.2005 (4)

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

Type	:	LC50
Value	:	300 mg/kg bw
Species	:	mouse
Strain	:	
Sex	:	
Number of animals	:	
Vehicle	:	
Doses	:	
Route of admin.	:	i.p.
Exposure time	:	
Method	:	
Year	:	1969
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	Mice were dosed intraperitoneal route. The observation period was at least 7 days. Any surviving animals were killed and dissected after this time. No further details given
Result	:	LD50: The median lethal dose of 3-methylbenzonitrile when administered to mice were 1400 mg/kg.
Reliability	:	(3) invalid 3a: Documentation insufficient for assessment

20.12.2005 (4)

5.2.1 SKIN IRRITATION

Species	:	rabbit
Concentration	:	
Exposure	:	
Exposure time	:	
Number of animals	:	
Vehicle	:	
PDII	:	
Result	:	slightly irritating
Classification	:	
Method	:	other: pad test
Year	:	1969
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	The test material was applied to the backs of white rabbits on 2.5 X 2.5 cm cotton pads. Each pad saturated with the test material was placed on the back for a period of 15 minutes of 20 hours. After the 15 minute application the area was washed with undiluted polyethyleneglycol 400 and then finally washed with a 50% solution of polyethyleneglycol 400; after the 20 hour treatment the skin was not washed. The skin reaction was observed immediately after pad removal and after 1, 3 and 8 days until the skin changes had disappeared.
Result	:	At 15 mins - slight vascular injection. At 20 hours - significant vascular injection.
Reliability	:	(3) invalid 3a: Documentation insufficient for assessment

20.12.2005 (4)

5.2.2 EYE IRRITATION

Species	:	rabbit
Concentration	:	
Dose	:	
Exposure time	:	
Comment	:	
Number of animals	:	
Vehicle	:	
Result	:	
Classification	:	irritating
Method	:	other: acute mucous membrane reaction
Year	:	1969
GLP	:	no
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	One drop of the test material (ca 50 mm3) was instilled into the conjunctival sac of the rabbit's eye and carefully spread over the upper eye. The reactions were noted after 10 minutes, 1 and 24 hours, 3 and 8 days and until the disappearance of any reaction.
Result	:	When administered to the rabbit eye 3-methylbenzonitrile caused necrosis. No further details given.
Reliability	:	(3) invalid 3a: Documentation insufficient for assessment

20.12.2005 (4)

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

(1) Cited as experimental in EPIWin Modeling Program. (version 3.12) 2000. Developed by the EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC). copyright 2000 U.S. Environmental Protection Agency

(2) EPIWin Modeling Program. (version 3.12) 2000. Developed by the EPA's Office of Pollution Prevention Toxics and Syracuse Research Corporation (SRC). copyright 2000 U.S. Environmental Protection Agency

(3) MSDS, m-Tolunitrile - 99%, revised 10 March 2005, supplied by Ficher Scientific.

(4) Zeller H et al, The toxicity of nitriles. Zentralblatt fur Areitsmedizin and Arbeitsschtz, 19(8) 225-238 1969

10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT